Propyl carbamate 627-12-3 | DTXSID7060833

Model Performance

- 1		Б .
	Model	I)ata
- 1	Wiodel	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 3.70e-01

Global applicability domain: Inside

Local applicability domain index: 6.43e-01

Confidence level: 7.06e-01

Nearest Neighbors from the Training Set

Image not found

Propyl carbamate Measured: 0.36 Predicted: 3.70e-01

Image not found

Carbamic acid, butyl ester

Measured: 0.85 Predicted: 8.43e-01

Image not found

Urethane

Measured: -0.150 Predicted: -0.120

Image not found

Carbamic acid, 2-methylpropyl

ester

Measured: 0.65 Predicted: 7.83e-01

Image not found

Acetoxime
Measured: 0.12
Predicted: 8.84e-01